Oxalyl chloride

Other names:	Ethanedioyl dichloride
	Ethanedioyl chloride
	Oxalic acid dichloride
	Oxalic dichloride
	Oxaloyl chloride
	Oxalyl dichloride
	(COCl)2
Inchi:	InChI=1S/C2Cl2O2/c3-1(5)2(4)6
InchiKey:	CTSLXHKWHWQRSH-UHFFFAOYSA-N
Formula:	C2Cl2O2
SMILES:	O=C(Cl)C(=O)Cl
Mol. weight [g/mol]:	126.93
CAS:	79-37-8

Physical Properties

Property code	Value	Unit	Source
chl	-417.00 ± 2.00	kJ/mol	NIST Webbook
gf	-315.74	kJ/mol	Joback Method
hf	-335.80 ± 6.30	kJ/mol	NIST Webbook
hfl	-367.60 ± 4.70	kJ/mol	NIST Webbook
hfus	12.53	kJ/mol	Joback Method
hvap	32.00 ± 4.00	kJ/mol	NIST Webbook
ie	10.91 ± 0.05	eV	NIST Webbook
ie	11.26	eV	NIST Webbook
ie	11.33	eV	NIST Webbook
log10ws	-0.52		Crippen Method
logp	0.517		Crippen Method
mcvol	66.660	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	427.76	K	Joback Method
tc	640.17	K	Joback Method
tf	272.00	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.14	J/mol×K	427.76	Joback Method
cpg	93.97	J/mol×K	463.16	Joback Method
cpg	96.63	J/mol×K	498.56	Joback Method
cpg	99.11	J/mol×K	533.97	Joback Method
cpg	101.43	J/mol×K	569.37	Joback Method
cpg	103.57	J/mol×K	604.77	Joback Method
cpg	105.55	J/mol×K	640.17	Joback Method
dvisc	0.0030801	Pa×s	272.00	Joback Method
dvisc	0.0020092	Pa×s	297.96	Joback Method
dvisc	0.0014035	Pa×s	323.92	Joback Method
dvisc	0.0010340	Pa×s	349.88	Joback Method
dvisc	0.0007947	Pa×s	375.84	Joback Method
dvisc	0.0006318	Pa×s	401.80	Joback Method
dvisc	0.0005165	Pa×s	427.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.70	K	102.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79378&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume